

The valence electron pair repulsion model (VSEPR) can be used with Lewis structure diagrams to predict the shapes of different molecules.

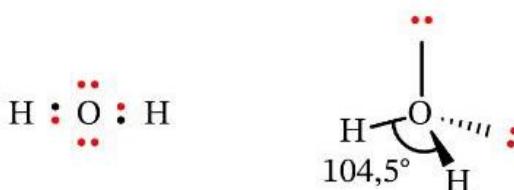
Lewis structure diagrams are used to identify valence electrons in polyatomic molecules, and the VSEPR model is used to understand how these valence electrons are arranged in three-dimensional space. The VSEPR model assumes that there will always be electrostatic repulsion between valence electron pairs. The valence electrons will be forced to adopt specific three-dimensional shapes that will minimize high-energy repulsive electrostatic interactions.

The  $AX_nE_m$  method is used with Lewis schemes to classify molecules and polyatomic ions into different groups. Each group has a preferred three-dimensional geometry. The term A represents the central atom, and the terms  $X_n$  and  $E_m$  represent the bonding and non-bonding pairs. The values of n and m are always integers, and they represent the number of bonding and non-bonding pairs.

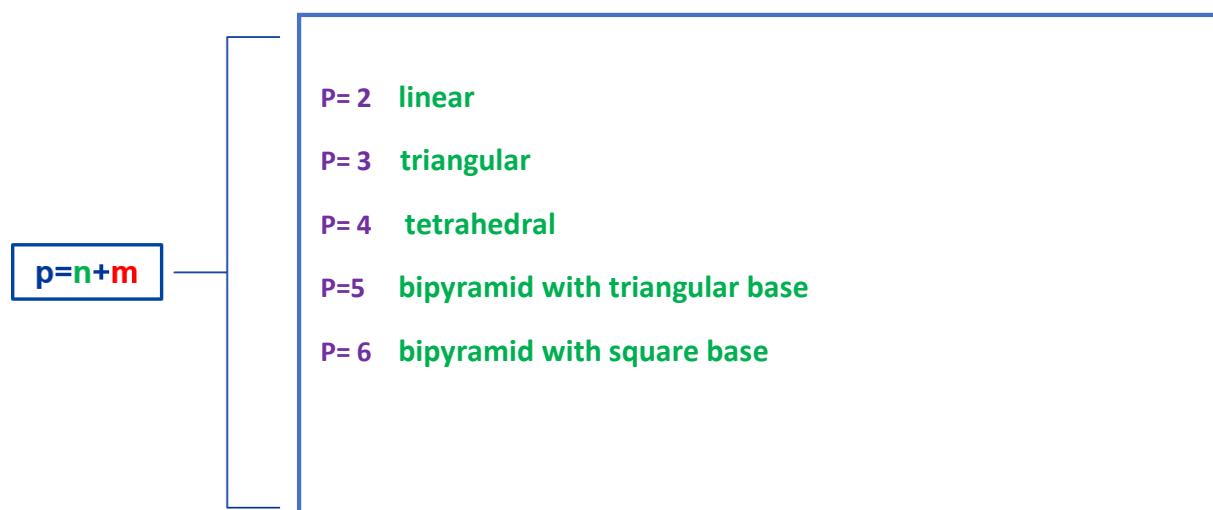
The non-bonding pairs occupy the most space in the valence shell of the central atom, and generate the strongest electrostatic repulsion interactions in the VSEPR model. The weakest electrostatic repulsion interactions are those between two bonding pairs. The combination of a non-bonding pair and a bonding pair has a force that lies between these two extremes.

Water molecules, for example, are able to dissolve polar alcohols and carboxylic acids in solution because they have a nonlinear or “bent” structure. They have an asymmetric distribution of electron density, and they have a permanent dipole moment which extends from the plane of the hydrogen atoms to the non-bonding doublets of oxygen. Lewis structure diagrams and the VSEPR model can be used to understand the shape of water molecules.

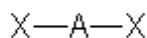
Structure de Lewis      Modèle VSEPR



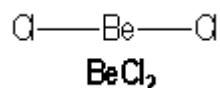
Sulfur dioxide is very soluble in water. Carbon dioxide is much less so. This difference in behavior on the macroscopic scale is interpreted on the microscopic scale by the different stereochemistries of the molecules. The  $CO_2$  and  $SO_2$  molecules each have two oxygen atoms bonded to a central atom. The infrared spectrum of  $CO_2$  is in favor of a linear molecule while that of  $SO_2$  shows that it has a bent shape. Thus, the dipole moment of  $SO_2$  is not zero, which allows it to interact with water, while that of  $CO_2$  is zero by compensating the bond dipole moments.



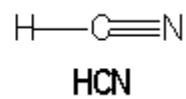
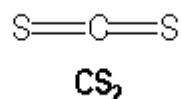
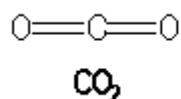
### Linear arrangement AX<sub>2</sub>



Beryllium, an element of the second column of the periodic table with electronic configuration [He]: 2s<sub>2</sub>, is linked by 2 single bonds to two chlorine atoms in the BeCl<sub>2</sub> molecule.

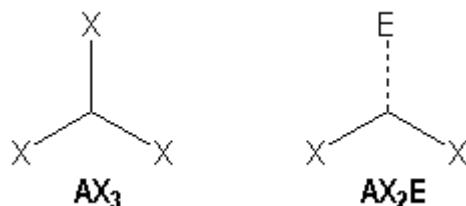


Molecules with multiple bonds :



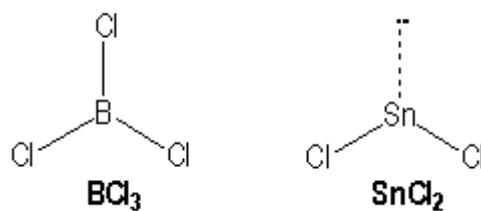
### Triangular arrangement AX<sub>3</sub>

We distinguish two families :



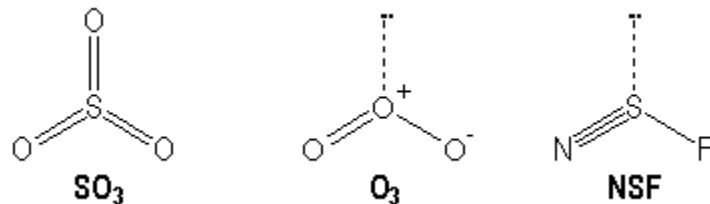
Molecules with simple bonds :

B	Sn
[He] 2s <sup>2</sup> 2p <sup>1</sup>	[Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup>



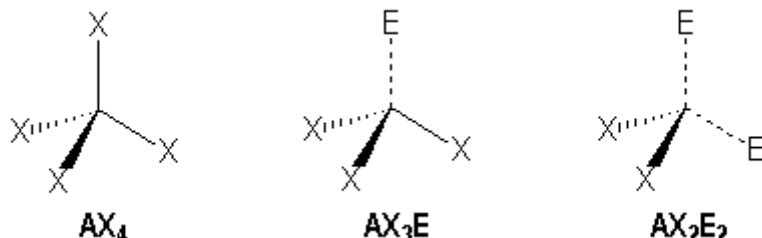
Molecules with multiple bonds :

S	O	N
$[\text{Ne}] 3s^2 3p^4$	$[\text{He}] 2s^2 2p^4$	$[\text{He}] 2s^2 2p^3$



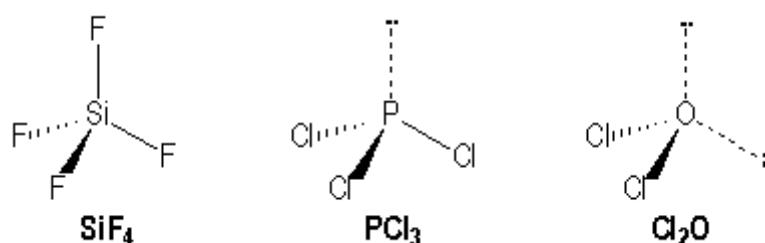
### Tetrahedral arrangement

We distinguish three families :



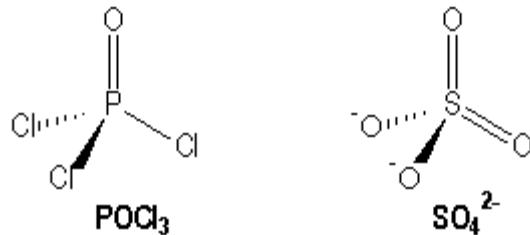
Molecules with simple bonds :

Si	P	O
$[\text{Ne}] 3s^2 3p^2$	$[\text{Ne}] 3s^2 3p^3$	$[\text{He}] 2s^2 2p^4$

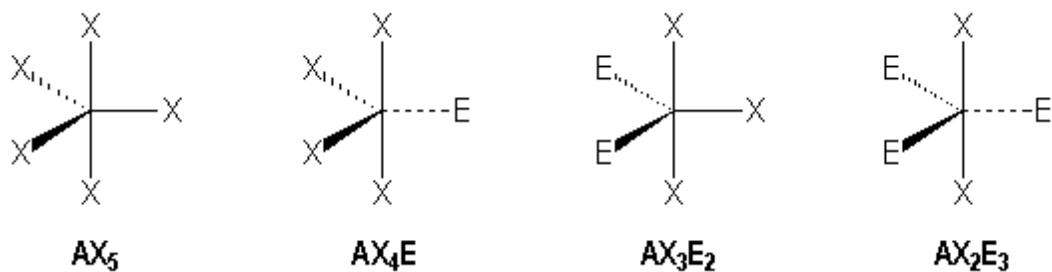


Molecules with multiple bonds :

P	S
[Ne] 3s <sup>2</sup> 3p <sup>1</sup>	[Ne] 3s <sup>2</sup> 3p <sup>4</sup>

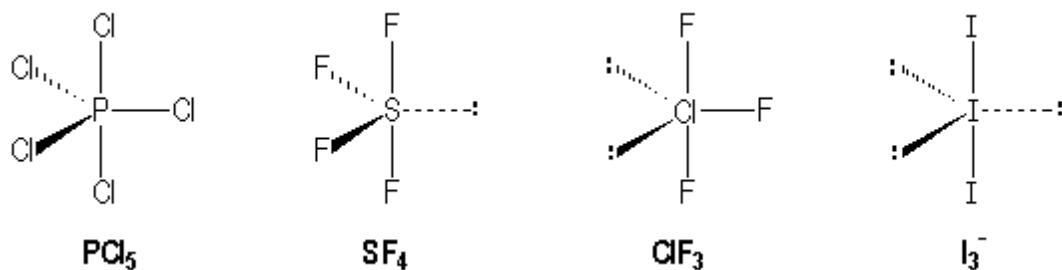


### Pentagonal arrangement : bipyramid with triangular base



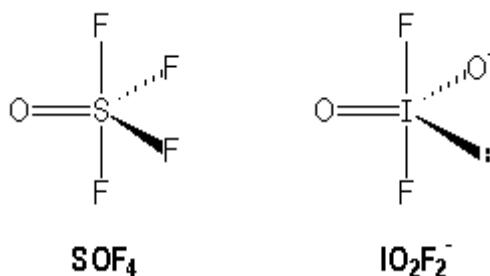
Molecules with simple bonds :

P	S	Cl	I
[Ne] 3s <sup>2</sup> 3p <sup>3</sup>	[Ne] 3s <sup>2</sup> 3p <sup>4</sup>	[Ne] 3s <sup>2</sup> 3p <sup>5</sup>	[Kr] 4 d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup>



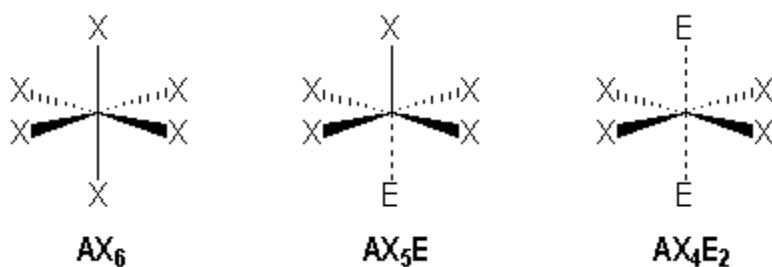
Molecules and ions with multiple bonds :

S	I
[Ne] 3s <sup>2</sup> 3p <sup>4</sup>	[Kr] 4 d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup>



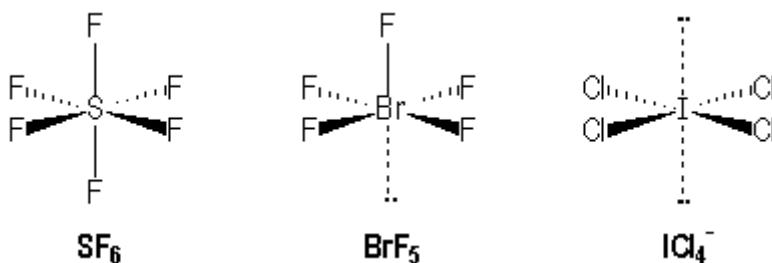
### Octahedral arrangement : bipyramid with square base

We distinguish the following families :



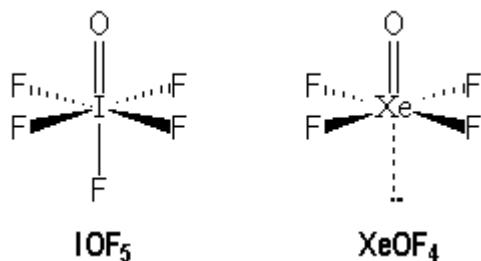
Molecules with simple bonds :

S	Br	I
[Ne] 3s <sup>2</sup> 3p <sup>4</sup>	[Kr] 3 d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup>	[Kr] 4 d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup>



Molecules with multiple bonds :

I	Xe
[Kr] 4 d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup>	[Kr] 4 d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup>



### Factors influencing angles between bonds

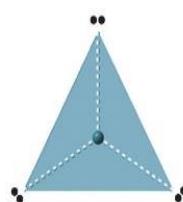
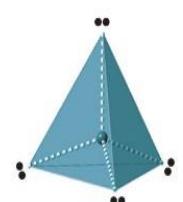
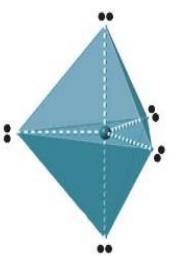
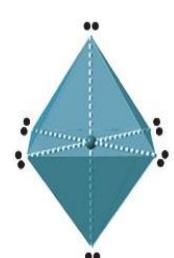
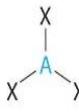
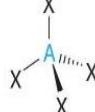
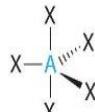
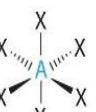
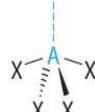
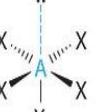
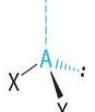
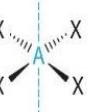
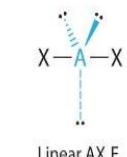
The nature of the pairs (bonding or non-bonding)

Multi-bond volume

The difference in electronegativity between atoms

### Limitations of the VSEPR method

The VSEPR method most of the time allows the correct prediction of the local arrangement of electron pairs around an atom when it can be unambiguously chosen as the central atom. On the other hand, its application is much more problematic when it comes to predicting the overall geometry of complex molecules.

Electron Groups	2	3	4	5	6
Molecular Geometry					
	Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
Zero Lone Pairs	$\text{X}-\text{A}-\text{X}$				
	Linear $\text{AX}_2$	Trigonal planar $\text{AX}_3$	Tetrahedral $\text{AX}_4$	Trigonal bipyramidal $\text{AX}_5$	Octahedral $\text{AX}_6$
One Lone Pair					
	Bent (V-shaped) $\text{AX}_2\text{E}$	Trigonal pyramidal $\text{AX}_3\text{E}$	Seesaw $\text{AX}_4\text{E}$ One axial lone pair	Square pyramidal $\text{AX}_5\text{E}$	
Two Lone Pairs					
	Bent (V-shaped) $\text{AX}_2\text{E}_2$	T-shaped $\text{AX}_3\text{E}_2$ Two axial lone pairs	Square planar $\text{AX}_4\text{E}_2$		
Three Lone Pairs					
			Linear $\text{AX}_2\text{E}_3$ Three axial lone pairs		